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Crystallization and defect formation in HfO_2 films on silicon. JACOB GAVARTIN, ALEXANDER SHLUGER, MARSHALL STONEHAM, University College London, GENNADI BERSUKER, SEMATECH — Hafnium dioxide currently is considered a dielectric of choice for novel MOSFET devices but it has an important drawback (as most high-k films on silicon) of low crystallization temperature. We use large scale plane wave density functional simulations of the $HfO_2/SiO_x/Si$ system to determine the properties of the amorphous hafnia films and the mechanisms of their crystallization and defects formation associated with it. We propose that the kinetics of interface formation stipulates some oxygen substoichiometry in hafnia. The resulting 'amorphous' films are characterized by the sub-coordinated (by less than 7 oxygen) Hf ions and some shortened Hf-Hf distance ($\sim$3 Å compared to $\sim$3.5 Å in the monoclinic HfO_2). Such structures may not have defect states (understood as localized states with energies in the band gap). However, they are characterized by the long band tails, whose origin will be discussed. Crystallization of such amorphous structures during thermal annealing results in the oxygen vacancy formation. We discuss the role of these vacancies in the trapping and de-trapping of carriers from the channel and the possibilities of control of their concentration.

Marshall Stoneham
University College London

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